Identification of Flame Edges from Multispecies Chemical Compositon Data

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Introduction

- Flames are loosely defined as a coupled multiscalar manifold.
- The multiscalar fields represent the chemical composition of the flame.
- In turbulent flows, the topology of this field changes dynamically.
- Typical hydrocarbon flames involve up to hundred of chemical species.
- The study of this complex geometrical object is important from the mathematical and physical point of view.

Computational Physics

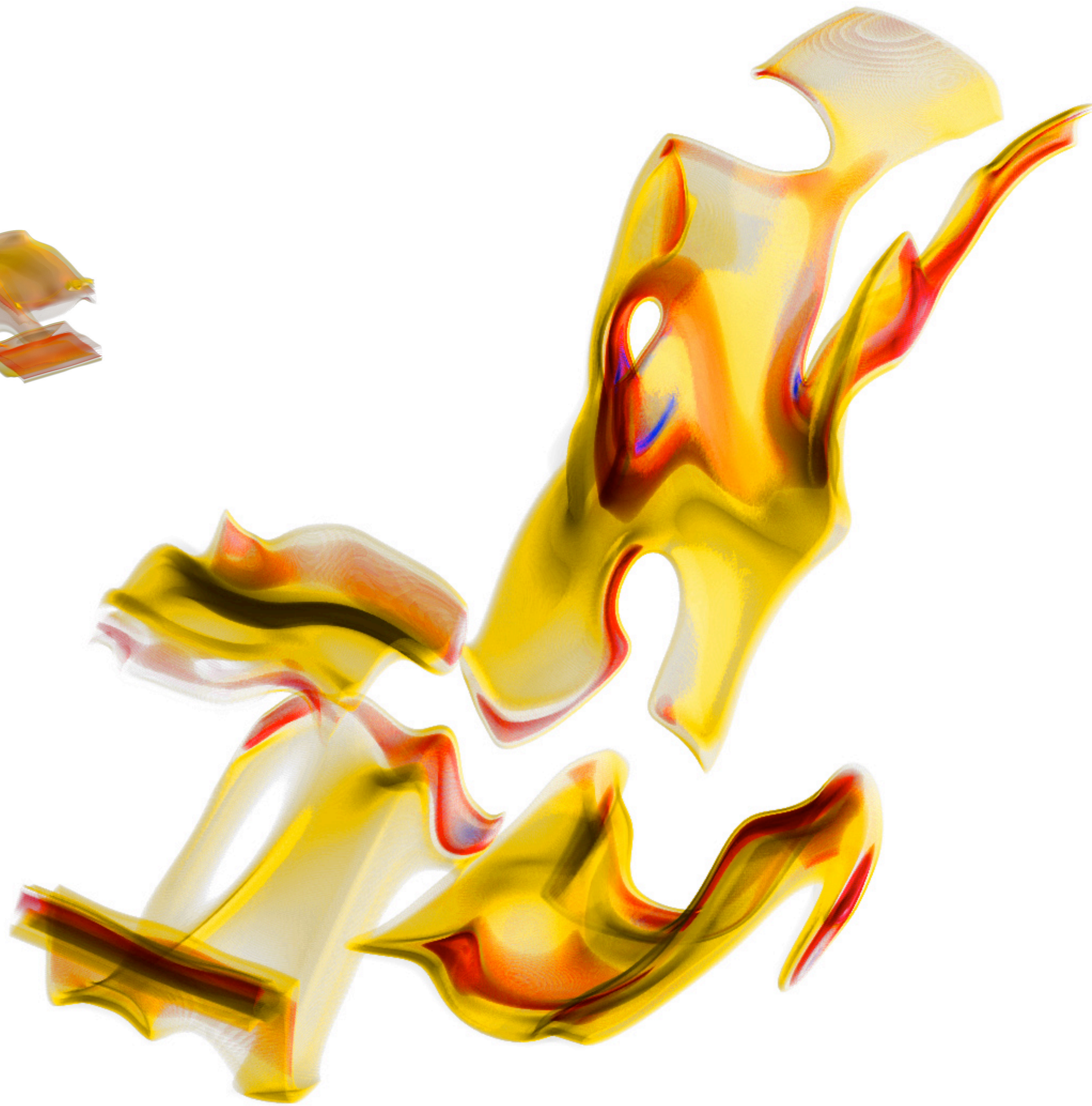
- We performed a Direct Numerical Simulation of a turbulent methane-air flame in the regime where extinction holes are observed.
- In this regime the flame is a complex percolated object.
- Chemistry is modeled by a reduced mechanism that involves 8 chemical species:

$$CH_4, O_2, H_2O, CO_2, CO, H_2, H, N_2$$

- No radiation and constant transport coefficients are used.

Database

- Compressible multispecies Navier-Stokes equations.
- 100 million grid points per field and time.
- 13 fields in the computation: 5 fluid mechanical and 8 chemical.
- Simulation time is approximately 4 months at Los Alamos National Laboratory's QSC.
- 6 TeraBytes of spatio-temporal and statistical data were generated.

Objectives

- Study the dynamics of partially extinguished flame manifolds
- In this regime, the burning and extinguished regions are separated by flame edges
- Understanding of their dynamics is a key issue in turbulent nonpremixed combustion
- First goal is to identify and extract the flame edges from the three dimensional dataset
- Once the edges are extracted, we need to determine the speed at which these edges travel

Tasks

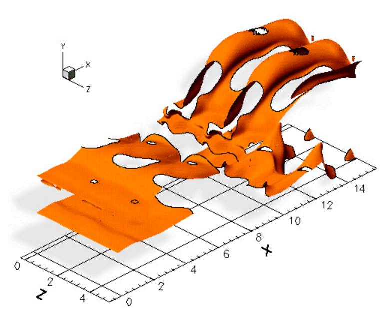
- The three objectives of this project are:
  1. Flame Edge Identification.
  2. Burning Flame area determination.
  3. Extraction of Flame Edge velocity statistics.

Flame Edge Identification

- There is no unique mathematical way to define the flame edges because multiple scalars are involved.
- We adopted a physically based approach in which edges are defined as the intersection of a hydrogen atom composition isosurface with the jet mixture fraction isosurface field (the fraction of jet to external fluid).
- Hydrogen atom composition is a good indication of the flame extent because it can only exit around the flame core (due to its reactivity).
- Our first problem is thus reduced to the determination of the intersection of two isosurfaces

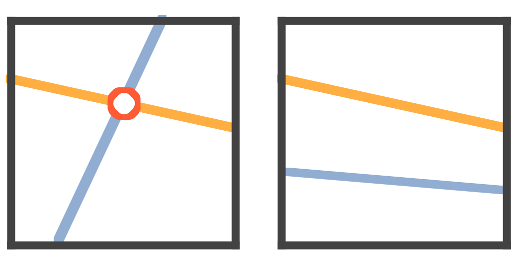
Concurrently Marching Cubes

- We adapted the *Marching Cubes* algorithm to work concurrently on two fields.
- Marching Cubes determines, at each voxel, the two set of surface triangulations corresponding to the two scalar fields.

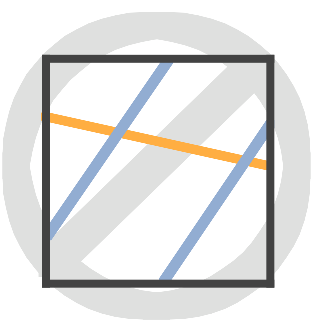


Edge Detection

- The flame edge detection is performed on the faces of the voxel.
- Each surface triangulation has at least one side on some of the surfaces of the voxel.
- Intersection of this 2D lines determine the nodal points of the flame edge.



Possible Cases



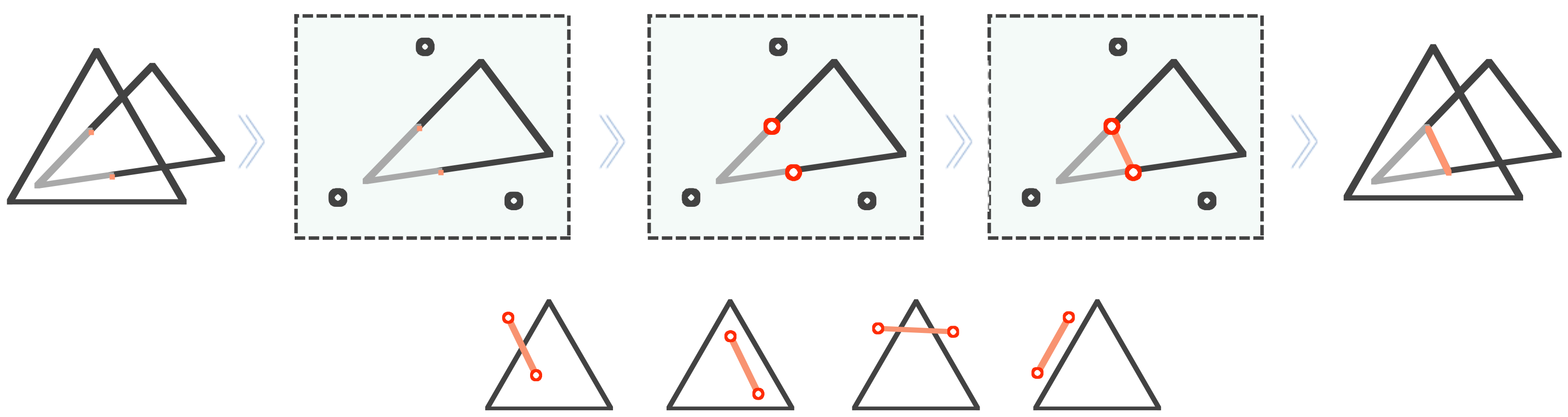
Non-Possible Cases

Edge Sorting

- Flame edges belong to two groups: edges that are closed forming holes and edges that are open due to intersection with the computational domain boundaries.
- The nodal edge locations are ordered based on a conditional bidirectional list traversal sorting algorithm.
- The condition for an edge to belong to the current active group is that its distance from the previous point is less than SQRT(3) on the unit side voxel.
- If no point is found, the current group is closed and a new group is opened.
- This is repeated until no original points are left.

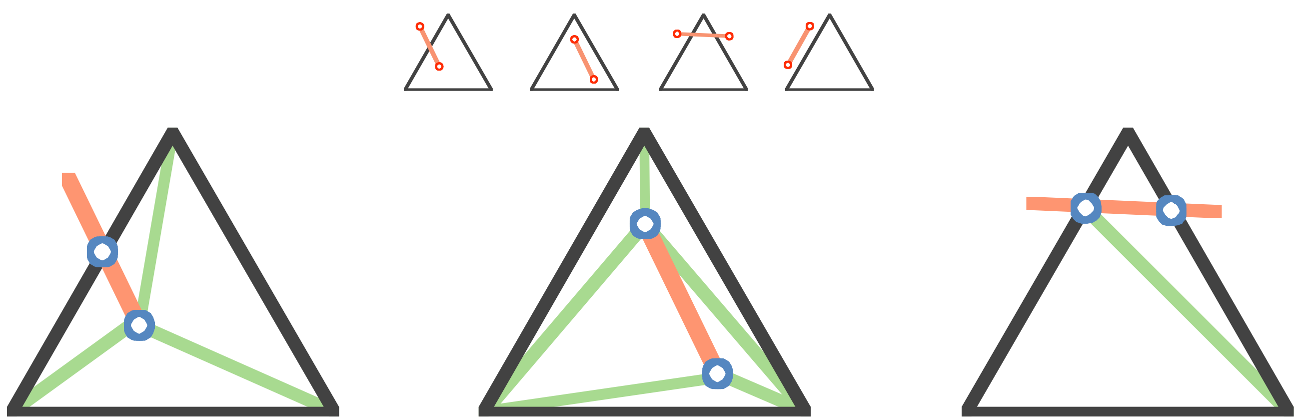
Burning Surface Area

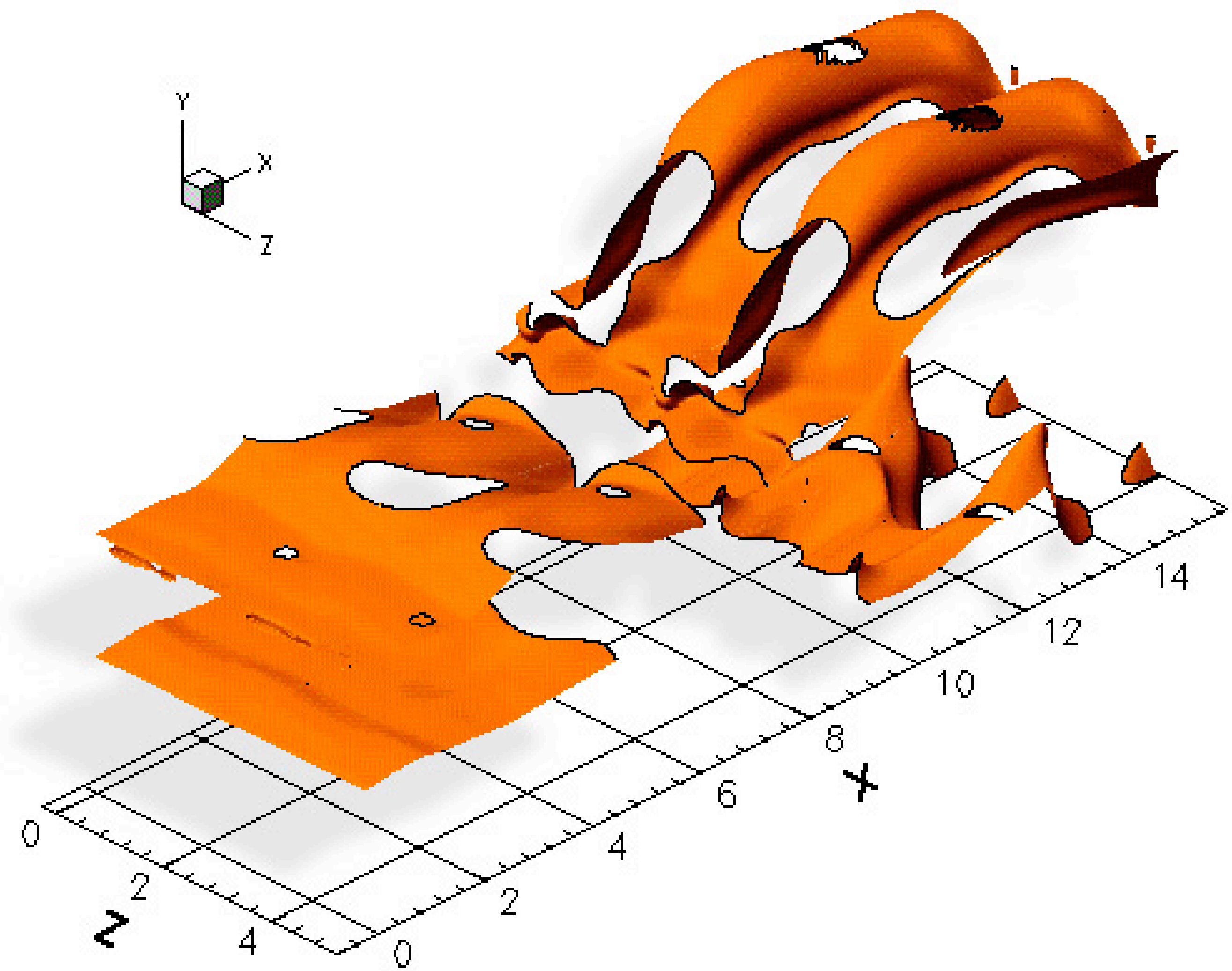
- The concurrent MCA is unable to determine if the two triangulations actually intersect within the voxel.
- An additional step is required to determine the true burning flame area.
- This is done by computing the intersection of each triangle on surface set A with the plane defined by the triangles in set B
- This intersection defines a line segment that can intersect the triangle in A or not.



Triangulation Subdivision

- In the cases where intersection is valid, the original triangle is subdivided in the corresponding two, tree or four subtriangles.
- The original triangle is removed from the list.
- The new subtriangles on the burning side are introduced to the triangle list.




Y
X
Z
0
2
4
Z
0
2
4
6
8
10
12
14
X

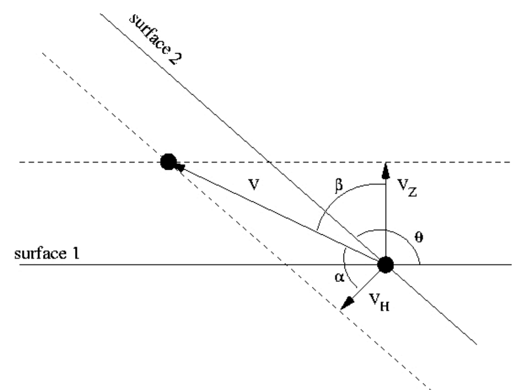
Flame Edge Velocity

- The edge velocity is determined from the edge location and the governing equations for the scalar fields.
- The normal isosurfaces velocity is given by:

$$V_Z = \vec{u} \cdot \vec{n}_Z - \frac{\nabla \cdot (\rho D_Z \nabla Z)}{\rho}$$

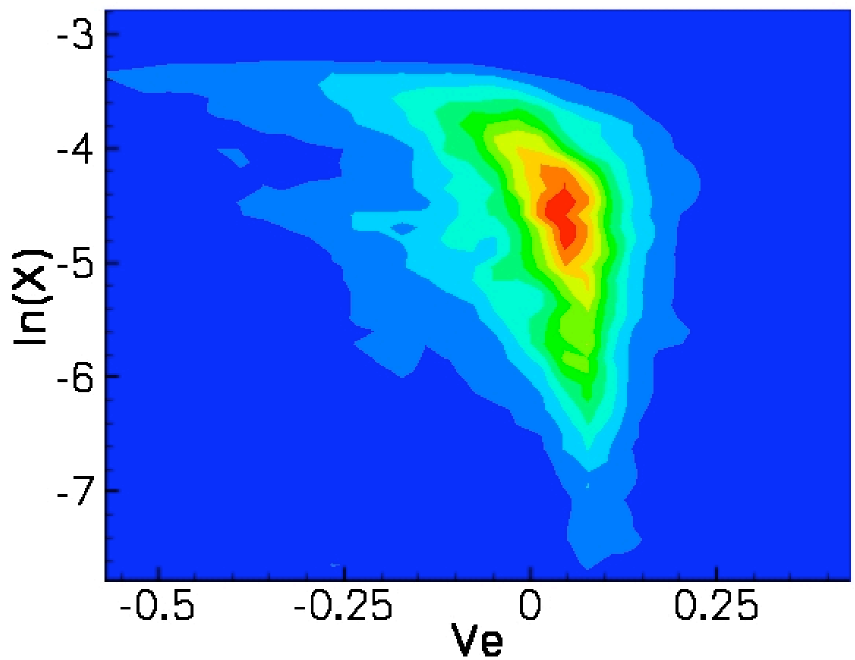
$$V_H = \vec{u} \cdot \vec{n}_H - \frac{\nabla \cdot (\rho D_H \nabla H) + \dot{\omega}_H}{\rho}$$

- The edge velocity is obtained from a geometric projection of the two surface velocities on the mixture fraction isosurface of set A.

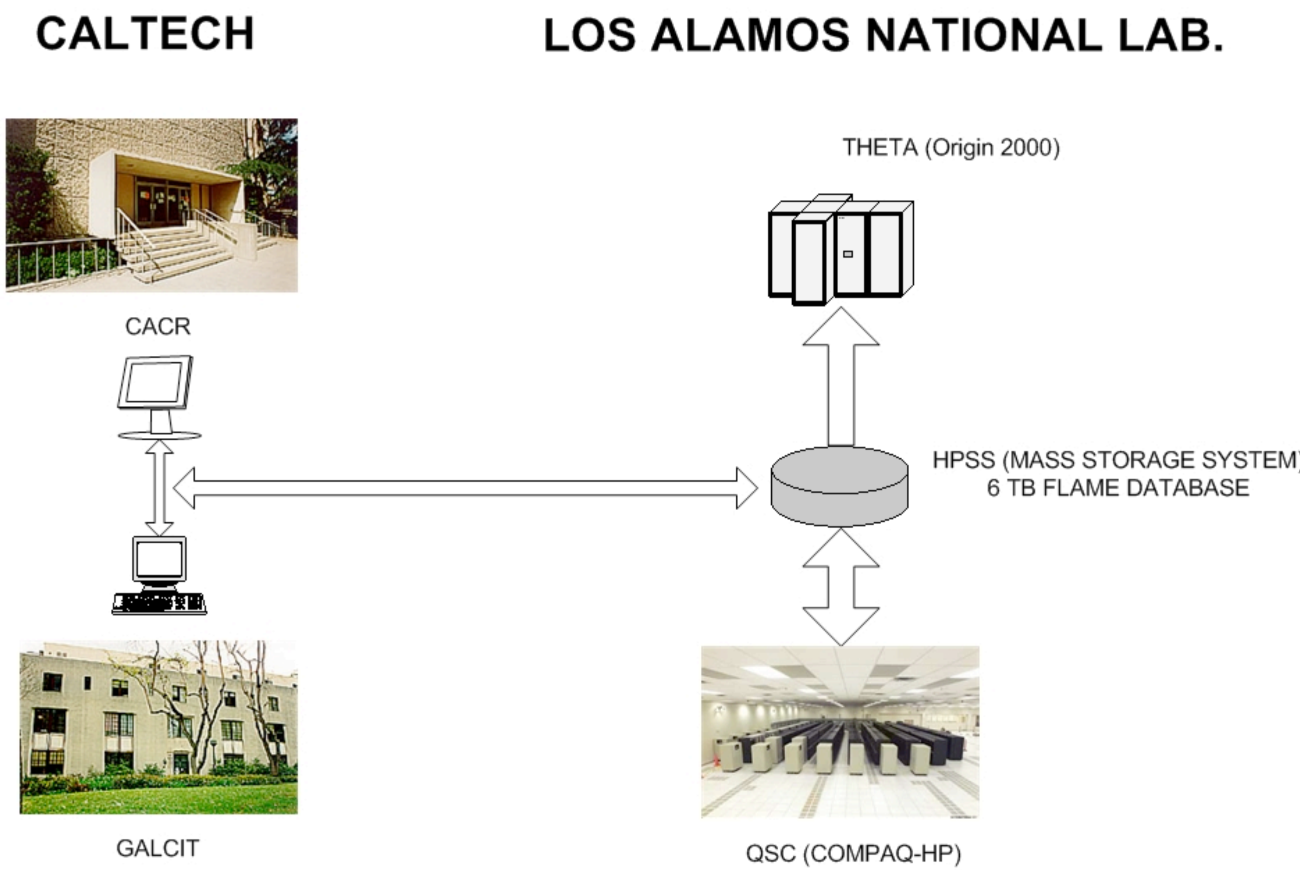


Physical Data

- Flame-edge velocity and mixture fraction gradient were extracted at multiple times and a joint probability distribution was constructed.



Computational and Visualization Resources



Algorithmic Performance

- The concurrently MCA with flame hole removal has approximately 10% overhead over the cost of 2 independent MCA (desirable).
  - ~ 30 seconds/frame on QSC.
- Edge identification is even faster due to the reduced dimensionality of the algorithm.
  - ~ 22 seconds/frame on QSC.
- Flame-edge velocity computation involves high order derivatives on the volumetric data and was done in parallel.
  - ~ 2 minutes/frame on THETA.
- Processing of 400 frames was done in a matter of hours.
- It took longer to get the database from HPSS.

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